

Predicting Shapes of Molecules

The Valence Shell Electron Pair Repulsion (VSEPR) theory is used to predict the 3D shape of molecules

- Proposed in 1957 by Ronald Gillespie, an English chemist working at McMaster
- Valence electrons around the central atom of a molecule determine shape
- The bonding pairs (BP) and the lone pairs (LP) around the central atom repel each other and arrange themselves in space so they are as far apart as possible
- A LP occupies more space than a BP since a BP is simultaneously attracted to 2 nuclei

Table Shapes of Molecules

No e ⁻ pairs around central	Chemical Formula	Lewis Structure	Around Central Atom		VESPR Notation	3D Arrangement	Name of Shape
			# BP	# LP			
4	CH ₄		4	0	AX ₄ OR AX ₄ E ₀		Tetrahedral
4	NH ₃		3	1	AX ₃ E ₁		Triangular/ Trigonal Pyramidal

No e ⁻ pairs around central	Chemical Formula	Lewis Structure	Around Central Atom		VSEPR Notation	3D Arrangement	Name of Shape
			# BP	# LP			
4	H ₂ O		2	2	AX ₂ E ₂		Bent/ angular
4	HCl		1	3	AXE ₃		Linear
5	PCl ₅		5	0	AX ₅		Trigonal Bipyramidal
5	SF ₄		4	1	AX ₄ E		Seesaw
5	ClF ₃		3	2	AX ₃ E ₂		T-shaped
5	XeF ₂		2	3	AX ₂ E ₃		Linear

No e ⁻ pairs around central	Chemical Formula	Lewis Structure	Around Central Atom		VESPR Notation	3D Arrangement	Name of Shape
			# BP	# LP			
6	OF ₆		6	0	AX ₆		Square Bipyramidal
6	BrF ₅		5	1	AX ₅ E		Square Pyramidal
6	XeF ₄		4	2	AX ₄ E ₂		Square Planar
3	BH ₃		3	0	AX ₃		Trigonal Planar
3	O ₃		2	1	AX ₂ E		V-shaped OR Bent
2	CS ₂		2	0	AX ₂		Linear

No e ⁻ pairs around central	Chemical Formula	Lewis Structure	Around Central Atom		VESPR Notation	3D Arrangement	Name of Shape
			# BP	# LP			
2	HCN		2	0	AX ₂		Linear
1	H ₂		1	0	A ₂		Linear
4	Cl ₂		1	3	A ₂ E ₆		Linear